

On solving symmetric systems of linear equations in an unnormalized Krylov subspace framework*

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Abstract

In an unnormalized Krylov subspace framework for solving symmetric systems of linear equations, the orthogonal vectors that are generated by a Lanczos process are not necessarily on the form of gradients. Associating each orthogonal vector with a triple, and using only the three-term recurrences of the triples, we give conditions on whether a symmetric system of linear equations is compatible or incompatible. In the compatible case, a solution is given and in the incompatible case, a certificate of incompatibility is obtained. In particular, the case when the matrix is singular is handled.

We also derive a minimum-residual method based on this framework and show how the iterates may be updated explicitly based on the triples, and in the incompatible case a minimum-residual solution of minimum Euclidean norm is obtained.

Keywords: Krylov subspace method, symmetric system of linear equations, unnormalized Lanczos vectors, minimum-residual method

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1. Introduction

An important problem in numerical linear algebra and optimization is to solve a system of equations where the matrix is symmetric. Such a problem may be posed as

$$Hx + c = 0, \quad (1.1)$$

for $x \in \mathbb{R}^n$, with $c \in \mathbb{R}^n$ and $H = H^T \in \mathbb{R}^{n \times n}$. Note that with $A = H$ and $b = -c$, (1.1) becomes $Ax = b$. However, we prefer the notation of (1.1) as it is on the form of a gradient g , defined as $g = Hx + c$, being equal to zero. This notation highlights that we are trying to find a non-trivial linear combination of the columns of H and c . Our primary motivation comes from optimization where in many cases the systems of linear equations that need to be solved are such that the matrix H is symmetric but in general indefinite. For example, KKT systems have this form, see, e.g., [8], but there are many other applications. Throughout, H is assumed symmetric, any

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other assumptions on H at particular instances will be stated explicitly. The key concept in this paper will be to determine if (1.1) is compatible or not. Our results include and handle the case when H is a singular matrix. It is assumed throughout that $c \neq 0$.

Exact arithmetic will be assumed and the theory developed in this paper is based on that assumption. In the end of the paper we briefly discuss computational aspects of our results in finite precision.

One strategy for solving (1.1) is to generate linearly independent vectors, q_k , $k = 0, 1, \dots$ until q_k becomes linearly dependent for some $k = r \leq n$ and hence $q_r = 0$. In this paper we consider Krylov subspace methods in which the generated vectors form an orthogonal, hence linearly independent, basis for the Krylov subspaces generated by H and c ,

$$\mathcal{K}_0(c, H) = \{0\}, \quad \mathcal{K}_k(c, H) = \text{span}\{c, Hc, H^2c, \dots, H^{k-1}c\}, \quad k = 1, 2, \dots \quad (1.2)$$

The Krylov vectors $c, Hc, \dots, H^{r-1}c$ are linearly independent, but as they become highly ill-conditioned it is desirable to work with some other set of vectors.

Orthogonal vectors q_k that are generated by a Lanczos process will be a linear combination of the columns of H and c . There is a freedom in the scaling of each generated vector. We will refer to the case when the coefficient corresponding to c is equal to one as a *normalized* Lanczos vector, i.e the vector is on the form of a gradient, $g = Hx + c$. An *unnormalized* Lanczos vector is then referring to the case when the coefficient corresponding to c is not required to be one, i.e. $q = Hy + \delta c$, where $\delta \in \mathbb{R}$.

The concept of using unnormalized Lanczos vectors was introduced by Gutknecht in [11, 12] as a remedy for so called pivot breakdowns that occur when normalization is not well defined.¹ In subsequent work by Gutknecht the term *inconsistent* is used, see, e.g., [13, 15]. However, in this paper the term unnormalized will be used as it better suits our purposes. The unnormalized framework will be used in a more general sense, not only as a remedy for pivot breakdown, to derive our results.

The Lanczos process was first introduced by Lanczos [18, 19]. There have been very many contributions to the theory both for symmetric and non-symmetric systems, see, e.g., Golub and O’Leary’s extensive survey of the years 1948-1976 [9], Golub and Van Loan’s book [10] and Gutknecht’s survey [13].

The outline of the paper is as follows. Section 2 gives a review of background material on the unnormalized Krylov subspace framework. In particular, we review recursions for the unnormalized Lanczos triples (q_k, y_k, δ_k) associated with the unnormalized Lanczos vectors q_k , $k = 0, \dots, r$, such that $q_k = Hy_k + \delta_k c$, $q_k \in \mathcal{K}_{k+1}(c, H)$, $y_k \in \mathcal{K}_k(c, H)$ and $\delta_k \in \mathbb{R}$, $k = 0, \dots, r$.

In Section 3, we give our main convergence result, based on the recursions for the triples, stating that when (1.1) is compatible a solution is given (in this case we show that $\delta_r \neq 0$), or a certificate of incompatibility can be obtained for (1.1) (in this case $\delta_r = 0$). The case of a singular matrix H is included and handled in the analysis,

¹Gutknecht considers the more general case when H is non symmetric where there are several other possible breakdowns for corresponding Lanczos a process, see, e.g., [13, 26]. For H symmetric, the pivot breakdown is the only one that can happen.

which to the best of our knowledge has not been done before. The derivation is summarized in an unnormalized Krylov algorithm, and in addition some remarks are made on the case when normalization is well defined and used.

Finally, in Section 4, a minimum-residual method, applicable also for incompatible systems, is derived by making use of the unnormalized Krylov framework. Explicit recursions for the minimum-residual iterates are derived, including an expression for the solution of minimum Euclidean norm in the incompatible case.

1.1. Notation

The letter i, j and k denote integer indices, other lowercase letters such as q, y and c denote column vectors, possibly with super- and/or subscripts. For a symmetric matrix H , $H \succ 0$ denotes that H is positive definite. Analogously, $H \succeq 0$ is used to denote that H is positive semidefinite. The null space and range space of H are denoted by $\mathcal{N}(H)$ and $\mathcal{R}(H)$ respectively. We will denote by Z an orthonormal matrix whose columns form a basis of $\mathcal{N}(H)$. If H is nonsingular, then Z is to be interpreted as an empty matrix. When referring to a norm, the Euclidean norm is used throughout.

2. Background

Regarding (1.1), the raw data available is the matrix H and the vector c and combinations of the two, for example represented by the Krylov subspaces generated by H and c , as defined in (1.2). For an introduction and background on Krylov subspaces, see, e.g., Gutknecht [14] and Saad [26].

Without loss of generality, the scaling of the first vector q_0 may be chosen so that $q_0 = c$. Then one sequence of linearly independent vectors may be generated by letting $q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp$, $k = 1, \dots, r$, such that $q_k \neq 0$, for $k = 0, 1, \dots, r-1$ and $q_r = 0$ where r is the minimum index k for which $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$. These vectors $\{q_0, q_1, \dots, q_{r-1}\}$ form an orthogonal, hence linearly independent, basis of $\mathcal{K}_r(c, H)$. We will refer to these vectors as the Lanczos vectors. With $q_0 = c$, each vector q_k , $k = 1, \dots, r-1$, is uniquely determined up to a scaling. A vector $q_k \in \mathcal{K}_{k+1}(c, H)$ may be expressed as

$$q_k = \sum_{j=0}^k \delta_k^{(j)} H^j c, \quad (2.1)$$

for some parameters $\delta_k^{(j)}$, $j = 0, \dots, k$, uniquely determined up to a nonzero scaling and $\delta_k^{(k)} \neq 0$. This is made precise in Lemma A.1.

Normalized Lanczos vectors are obtained when the scaling is chosen such that $\delta_k^{(0)} = 1$, and we call this the normalization condition.² Since $\delta_k^{(0)}$ is determined up to a scaling it holds that if $\delta_k^{(0)} \neq 0$ then one can rescale the vector such that the

²From (2.1), one can see that the vectors q_k may be represented as $q_k = p_k(H)c$, where p_k is polynomial of degree k , hence the normalization condition may be stated as $p_k(0) = 1$, see, e.g., Gutknecht [13]

normalization condition holds, however if $\delta_k^{(0)} = 0$, then this is not possible and a pivot breakdown occurs.

The following proposition reviews a recursion for a sequence of Lanczos vectors where the scaling factors denoted by $\{\theta_k\}_{k=0}^{r-1}$ are left unspecified. This recursion is a slight generalization of the symmetric Lanczos process for generating mutually orthogonal vectors, in which the usual choice of the scaling is such that each vector q_k is chosen such that $\|q_k\| = 1$, $k = 0, \dots, r-1$. For completeness, this proposition and its proof is included.

Proposition 2.1. *Let r denote the smallest positive integer k for which $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$. Given $q_0 = c \in \mathcal{K}_1(c, H)$, there exist vectors q_k , $k = 1, \dots, r$, such that*

$$q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp, \quad k = 1, \dots, r,$$

for which $q_k \neq 0$, $k = 1, \dots, r-1$, and $q_r = 0$. Each such q_k , $k = 1, \dots, r-1$, is uniquely determined up to a scaling, and a sequence $\{q_k\}_{k=1}^r$ may be generated as

$$q_1 = \theta_0 \left(-Hq_0 + \frac{q_0^T H q_0}{q_0^T q_0} q_0 \right), \quad (2.2a)$$

$$q_{k+1} = \theta_k \left(-Hq_k + \frac{q_k^T H q_k}{q_k^T q_k} q_k + \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} q_{k-1} \right), \quad k = 1, \dots, r-1, \quad (2.2b)$$

where θ_k , $k = 0, \dots, r-1$, are free and nonzero parameters. In addition, it holds that

$$q_{k+1}^T q_{k+1} = -\theta_k q_{k+1}^T H q_k, \quad k = 0, \dots, r-1. \quad (2.3)$$

Proof. Given $q_0 = c$, let k be an integer such that $1 \leq k \leq r-1$. Assume that q_i , $i = 0, \dots, k$, are mutually orthogonal with $q_i \in \mathcal{K}_{i+1}(c, H) \cap \mathcal{K}_i(c, H)^\perp$. Let $q_{k+1} \in \mathcal{K}_{k+2}(c, H)$ be expressed as

$$q_{k+1} = -\theta_k H q_k + \sum_{i=0}^k \eta_k^{(i)} q_i, \quad k = 0, \dots, r-1, \quad (2.4)$$

In order for q_{k+1} to be orthogonal to q_i , $i = 0, \dots, k$, the parameters $\eta_k^{(i)}$, $i = 0, \dots, k$, are uniquely determined as follows.

For $k = 0$, to have $q_0^T q_1 = 0$, it must hold that

$$\eta_0^{(0)} = \theta_0 \frac{q_0^T H q_0}{q_0^T q_0},$$

hence obtaining $q_1 \in \mathcal{K}_2(c, H) \cap \mathcal{K}_1(c, H)^\perp$ as in (2.2a), where θ_0 is free and nonzero. For k such that $1 \leq k \leq r-1$, in order to have $q_i^T q_{k+1} = 0$, $i = 0, \dots, k$, it must hold that

$$\eta_k^{(k)} = \theta_k \frac{q_k^T H q_k}{q_k^T q_k}, \quad \eta_k^{(k-1)} = \theta_k \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}}, \quad \text{and} \quad \eta_k^{(i)} = 0, \quad i = 0, \dots, k-2.$$

The last relation follows by the symmetry of H . Hence, obtaining $q_{k+1} \in \mathcal{K}_{k+2}(c, H) \cap \mathcal{K}_{k+1}(c, H)^\perp$ as in the three-term recurrence of (2.2b), where θ_k , $k = 1, \dots, r-1$, are free and nonzero.

Since q_1 is orthogonal to q_0 , and since q_{k+1} is orthogonal to q_k and q_{k-1} , $k = 1, \dots, r-1$, pre-multiplication of (2.2) with q_{k+1}^T yields

$$q_{k+1}^T q_{k+1} = -\theta_k q_{k+1}^T H q_k, \quad k = 0, \dots, r-1.$$

Finally note that if q_{k+1} is given by (2.2), then the only term that increases the power of H is $\theta_k(-Hq_k)$. Since $\theta_k \neq 0$, repeated use of this argument gives $\delta_{k+1}^{(k+1)} \neq 0$ if q_{k+1} is expressed by (2.1). In fact, $\delta_{k+1}^{(k+1)} = (-1)^{k+1} \prod_{i=0}^k \theta_i \neq 0$. Hence, by Lemma A.1, $q_{k+1} = 0$ implies $\mathcal{K}_{k+2}(c, H) = \mathcal{K}_{k+1}(c, H)$, so that $k+1 = r$, as required. ■

The particular form of (2.2) with scaling parameters θ_k , $k = 0, \dots, r$, is made to get coherence with existing theory on the method of conjugate gradients, see Section 3.3 and Proposition A.6. To simplify the exposition, the following notation is introduced,

$$\alpha_0 = \frac{q_0^T H q_0}{q_0^T q_0}, \quad \alpha_k = \frac{q_k^T H q_k}{q_k^T q_k}, \quad \beta_{k-1} = \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} \quad k = 1, \dots, r-1. \quad (2.5)$$

Let Q_k be the matrix with the Lanczos vectors q_0, q_1, \dots, q_k as columns vectors, then (2.2) may be written on matrix form as,

$$H Q_k = Q_{k+1} \bar{T}_k = Q_k T_k - \frac{1}{\theta_k} q_{k+1} e_{k+1}^T,$$

where

$$T_k = \begin{pmatrix} \alpha_0 & \beta_0 & & \\ -\frac{1}{\theta_0} & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ & & -\frac{1}{\theta_{k-1}} & \alpha_k \end{pmatrix}, \quad \bar{T}_k = \begin{pmatrix} T_k \\ -\frac{1}{\theta_k} e_{k+1}^T \end{pmatrix}. \quad (2.6)$$

The choice of θ_k such that $\|q_k\|_2 = \|q_0\|_2$ implies $\beta_k = -\frac{1}{\theta_k}$ and in this case T_k will be symmetric. Changing the set of $\{\theta_k\}_{k=0}^{r-1}$ can be seen as a similarity transform of T_k , see, e.g., Gutknecht [13].

Many methods for solving (1.1) use matrix-factorization techniques on T_k or \bar{T}_k . For an introduction to how Krylov subspace methods are formalized in this way, see, e.g., Paige, Saunders and Choi [5, 23]. For our purposes we leave these available scaling factors unspecified and work with the recursions (2.2) directly.

2.1. An extended representation of the unnormalized Lanczos vectors

To find a solution of (1.1), if it exists, it is not sufficient to generate the sequence $\{q_k\}_{k=1}^r$. Note that, as in (2.1), $q_k \in \mathcal{K}_{k+1}(c, H)$, $k = 0, \dots, r$, may be expressed as

$$q_k = \sum_{j=0}^k \delta_k^{(j)} H^j c = H \left(\sum_{j=1}^k \delta_k^{(j)} H^{j-1} c \right) + \delta_k^{(0)} c, \quad k = 1, \dots, r. \quad (2.7)$$

It is not convenient to represent q_k by (2.1). Therefore, defining $y_0 = 0$, $\delta_0 = 1$,

$$y_k = \sum_{j=1}^k \delta_k^{(j)} H^{j-1} c \in \mathcal{K}_k(c, H) \quad \text{and} \quad \delta_k = \delta_k^{(0)}, \quad k = 1, \dots, r,$$

it follows from (2.7) that

$$q_k = Hy_k + \delta_k c,$$

so that q_k may be expressed by y_k and δ_k . These quantities will be represented by the triples (q_k, y_k, δ_k) , $k = 0, \dots, r$. Note that $\{\delta_k^{(j)}\}_{j=0}^k$ are given in association with the raw data H and c , the choice made here is to use only $\delta_k^{(0)}$ explicitly and collect all other terms in y_k .

It is straightforward to note that if $\delta_r \neq 0$, then $0 = q_r = Hx_r + c$ for $x_r = (1/\delta_r)y_r$, so that x_r solves (1.1). It will be shown that (1.1) has a solution if and only if $\delta_r \neq 0$.

As mentioned earlier, for a given k such that $1 \leq k \leq r$, the parameters $\delta_k^{(j)}$, $j = 1, \dots, k$, are uniquely defined up to a scaling. Hence, so is the triple (q_k, y_k, δ_k) . This is made precise in the recursions for the triples given in Lemma 2.2.

It is possible to use more of the coefficients $\{\delta_k^{(j)}\}_{j=1}^k$ explicitly in the same representation as above. For the next power of the polynomial in (2.7), let

$$\begin{aligned} y_k &= Hy_k^{(1)} + \delta_k^{(1)} c, \quad \text{with} \\ y_k^{(1)} &= \sum_{j=2}^k \delta_k^{(j)} H^{j-2} c \in \mathcal{K}_{k-1}(c, H), \quad k = 2, \dots, r, \end{aligned} \tag{2.8}$$

in addition to $y_1^{(1)} = 0$. This will be used in the analysis, but not in the algorithm presented.

Based on Proposition 2.1, given $(q_0, y_0, \delta_0) = (c, 0, 1)$, one can formulate recursions for (q_k, y_k, δ_k) , $k = 1, \dots, r$. This derivation is given by Gutknecht in e.g. [13], but we give the following lemma for completeness.

Lemma 2.2. *Let r denote the smallest positive integer k for which $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$. Given $(q_0, y_0, \delta_0) = (c, 0, 1)$, there exist vectors (q_k, y_k, δ_k) , $k = 1, \dots, r$, such that*

$$q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp, \quad y_k \in \mathcal{K}_k(c, H), \quad q_k = Hy_k + \delta_k c, \quad k = 1, \dots, r,$$

for which $q_k \neq 0$, $k = 1, \dots, r-1$, and $q_r = 0$. Each such (q_k, y_k, δ_k) , $k = 1, \dots, r$, is uniquely determined up to a scalar, and a sequence $\{(q_k, y_k, \delta_k)\}_{k=1}^r$ may be generated as

$$y_1 = \theta_0(-q_0 + \alpha_0 y_0), \quad \delta_1 = \theta_0(\alpha_0 \delta_0), \quad q_1 = \theta_0(-Hq_0 + \alpha_0 q_0),$$

and

$$\begin{aligned} y_{k+1} &= \theta_k(-q_k + \alpha_k y_k + \beta_{k-1} y_{k-1}), & k &= 1, \dots, r-1, \\ \delta_{k+1} &= \theta_k(\alpha_k \delta_k + \beta_{k-1} \delta_{k-1}), & k &= 1, \dots, r-1, \\ q_{k+1} &= \theta_k(-Hq_k + \alpha_k q_k + \beta_{k-1} q_{k-1}), & k &= 1, \dots, r-1, \end{aligned}$$

where θ_k , $k = 0, \dots, r-1$, are free and nonzero parameters, and α_k , $k = 0, \dots, r-1$ and β_{k-1} , $k = 1, \dots, r-1$ are given by (2.5). In addition, it holds that y_k are linearly independent for $k = 1, \dots, r$.

Proof. The recursions are given by simple induction on k . We omit the details, see, e.g. [13].

By Lemma A.1 it holds that for $k = 0, \dots, r$, $\delta_k^{(j)}$, $j = 0, \dots, k$ are uniquely determined up to a scaling, hence it follows that y_{k+1} and δ_{k+1} , $k = 0, \dots, r-1$ are uniquely determined up to a scaling by the recursions of this proposition.

Further, note that the recursion for y_{k+1} has a nonzero leading term of q_k plus additional terms of y_i , $i = k$ and $i = k-1$. Since q_k is orthogonal to y_i for $i \leq k$ and $q_k \neq 0$ for $k < r$, it follows that the vectors y_{k+1} are linearly independent for $k = 0, \dots, r-1$. ■

Note that the choice

$$\theta_0 = \frac{1}{\alpha_0}, \quad \theta_k = \frac{1}{\alpha_k + \beta_{k-1}}, \quad k = 1, \dots, r-1, \quad (2.9)$$

in the recursions of Lemma 2.2 implies $\delta_k = 1$, $k = 0, \dots, r$. Hence, this choice will give rise to Lanczos vectors that are on the form of gradients. The terms g_k and x_k are reserved for this case, and we then denote (q_k, y_k, δ_k) by $(g_k, x_k, 1)$. Therefore, (2.9) is another way of stating the normalization condition. Note that if $\alpha_k + \beta_{k-1} = 0$, for some k , then this particular choice is not well defined and a pivot breakdown occurs. In the unnormalized Krylov subspace framework the choice of scaling will not be based on the value of δ_k .

3. Properties of the unnormalized Krylov framework

We will henceforth refer to the unnormalized Lanczos triples (q_k, y_k, δ_k) , $k = 0, \dots, r$, as given by Lemma 2.2. Based on the unnormalized framework due to Gutknecht that has been described in the previous section we will now proceed to state our results.

3.1. Convergence in the unnormalized Krylov framework

The final triple, (q_r, y_r, δ_r) , can now be used to show our main convergence result, namely that (1.1) has a solution if and only if $\delta_r \neq 0$, and that the recursions in Lemma 2.2 can be used to find a solution if $\delta_r \neq 0$ and a certificate of incompatibility if $\delta_r = 0$. The case when H is singular is included and handled in this result.

Theorem 3.1. *Let (q_k, y_k, δ_k) , $k = 0, \dots, r$, be given by Lemma 2.2, and let Z denote a matrix whose columns form an orthonormal basis for $\mathcal{N}(H)$. Then, the following holds for the cases $\delta_r \neq 0$ and $\delta_r = 0$ respectively.*

- a) *If $\delta_r \neq 0$, then $Hx_r + c = 0$ for $x_r = (1/\delta_r)y_r$, so that $c \in \mathcal{R}(H)$ and x_r solves (1.1). In addition, it holds that $Z^T y_k = 0$, $k = 0, \dots, r$.*

b) If $\delta_r = 0$, then $y_r = \delta_r^{(1)} Z Z^T c$, with $\delta_r^{(1)} \neq 0$ and $Z^T c \neq 0$, so that $c \notin \mathcal{R}(H)$ and (1.1) has no solution. Further, there is a $y_r^{(1)} \in \mathcal{K}_{k-1}(c, H)$ so that $y_r = H y_r^{(1)} + \delta_r^{(1)} c$. Hence, $H(H x_r^{(1)} + c) = 0$ for $x_r^{(1)} = (1/\delta_r^{(1)}) y_r^{(1)}$, so that $x_r^{(1)}$ solves $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$.

Proof. For (a), suppose that $\delta_r \neq 0$. Then $0 = q_r = H y_r + \delta_r c$, hence $H x_r + c = 0$ for $x_r = (1/\delta_r) y_r$, i.e., $x_r = (1/\delta_r) y_r$ is a solution to (1.1). Since (1.1) has a solution, it must hold that $Z^T c = 0$. We have $y_k = H y_k^{(1)} + \delta_k^{(1)} c$ for $k = 0, \dots, r$, so that $Z^T y_k = \delta_k^{(1)} Z^T c$. As $Z^T c = 0$, it follows that $Z^T y_k = 0$, $k = 0, \dots, r$.

For (b), suppose that $\delta_r = 0$. We have $y_r = H y_r^{(1)} + \delta_r^{(1)} c$, so that $Z^T y_r = \delta_r^{(1)} Z^T c$. If $\delta_r = 0$, then $0 = q_r = H y_r$ so that $y_r = \delta_r^{(1)} Z Z^T c$. It follows from Proposition 2.2 that $y_r \neq 0$ so that $\delta_r^{(1)} \neq 0$ and $Z^T c \neq 0$. A combination of $H y_r = 0$ and $y_r = H y_r^{(1)} + \delta_r^{(1)} c$ gives $H(H y_r^{(1)} + \delta_r^{(1)} c) = 0$. Consequently, since $\delta_r^{(1)} \neq 0$, it holds that $H(H x_r^{(1)} + c) = 0$ for $x_r^{(1)} = (1/\delta_r^{(1)}) y_r^{(1)}$. With $f(x) = \frac{1}{2} \|Hx + c\|_2^2$, one obtains $\nabla f(x) = H(Hx + c)$, so that $x_r^{(1)}$ is a global minimizer to f over \mathbb{R}^n . ■

Hence, we have shown that (1.1) has a solution if and only if $\delta_r \neq 0$, and that the recursions in Lemma 2.2 can be used to find a solution if $\delta_r \neq 0$ and a certificate of incompatibility if $\delta_r = 0$.

We can make a few comments on the sequence $\{\delta_k\}$. One can show that the sequence will never have two zero element in a row.³ Also, if θ_{k-1} and θ_k have the same sign and $\delta_k = 0$, then $\delta_{k+1} \delta_{k-1} < 0$. We give direct proofs of these properties, using only the recursions of the triples, in Appendix A.2.

3.2. An unnormalized Krylov algorithm

To summarize the derivation up to this point we now state an algorithm for solving (1.1) based on the triples (q_k, y_k, δ_k) , $k = 0, \dots, r$, given by Lemma 2.2 using some θ_k of our choice. Algorithm 3.1 is called a unnormalized Krylov algorithm⁴ as it is the unnormalized vectors $\{q_k\}$, spanning the Krylov subspaces, that drive the progress of the algorithm.

In the unnormalized setting, the choice of a nonzero θ_k is in theory arbitrary, but for the algorithm stated below we have made the choice to let $\theta_k > 0$ such that $\|y_{k+1}\|_2 = \|c\|_2$. This choice is well defined since $y_k \neq 0$, $k = 1, \dots, r$, by Lemma 2.2.

In theory, triples are generated as long as $q_k \neq 0$. In the algorithm, we introduce a tolerance such that the iterations proceed as long as $\|q_k\|_2 > q_{tol}$, where we let $q_{tol} = \sqrt{\epsilon_M}$, where ϵ_M is the machine precision. In theory, we also draw conclusions based on $\delta_r \neq 0$ or $\delta_r = 0$, for this we introduce a tolerance $\delta_{tol} = \sqrt{\epsilon_M}$.

By Theorem 3.1, Algorithm 3.1 will return either a solution to (1.1) or a certificate that the system is incompatible.

³This property is used in composite step biconjugate gradient method and other look-ahead techniques to show that a composite step or look-ahead block of size two is sufficient to avoid breakdown, see, e.g., [2, 4].

⁴In the terminology of Gutknecht's survey, [13], this method would be called inconsistent ORes version of the method of conjugate gradients.

Algorithm 3.1 An unnormalized Krylov algorithm

Input arguments: H, c ;
 Output arguments: compatible; x_r if compatible=1; y_r if compatible=0;
 $q_{tol} \leftarrow$ tolerance on $\|q\|_2$; [Our choice: $q_{tol} = \sqrt{\epsilon_M}$]
 $\delta_{tol} \leftarrow$ tolerance on $|\delta|$; [Our choice: $\delta_{tol} = \sqrt{\epsilon_M}$]
 $k \leftarrow 0$; $q_0 \leftarrow c$; $y_0 \leftarrow 0$; $\delta_0 \leftarrow 1$;
 $\alpha_0 \leftarrow \frac{q_0^T H q_0}{q_0^T q_0}$;
 $q_1 \leftarrow (-Hq_0 + \alpha_0 q_0)$; $y_1 \leftarrow (-q_0 + \alpha_0 y_0)$; $\delta_1 \leftarrow (\alpha_0 \delta_0)$;
 $\theta_0 \leftarrow$ nonzero scalar; [Our choice: $\theta_0 = \|c\|_2 / \|y_1\|_2$]
 $q_1 \leftarrow \theta_0 q_1$; $y_1 \leftarrow \theta_0 y_1$; $\delta_1 \leftarrow \theta_0 \delta_1$;
 $k \leftarrow 1$;
while $\|q_k\|_2 > q_{tol}$ **do**
 $\alpha_k \leftarrow \frac{q_k^T H q_k}{q_k^T q_k}$; $\beta_{k-1} \leftarrow \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}}$;
 $q_{k+1} \leftarrow (-Hq_k + \alpha_k q_k + \beta_{k-1} q_{k-1})$;
 $y_{k+1} \leftarrow (-q_k + \alpha_k y_k + \beta_{k-1} y_{k-1})$; $\delta_{k+1} \leftarrow (\alpha_k \delta_k + \beta_{k-1} \delta_{k-1})$;
 $\theta_k \leftarrow$ nonzero scalar; [Our choice: $\theta_k = \|c\|_2 / \|y_{k+1}\|_2$]
 $q_{k+1} \leftarrow \theta_k q_{k+1}$; $y_{k+1} \leftarrow \theta_k y_{k+1}$; $\delta_{k+1} \leftarrow \theta_k \delta_{k+1}$;
 $k \leftarrow k + 1$;
end while
 $r \leftarrow k$;
if $|\delta_r| > \delta_{tol}$ **then**
 $x_r \leftarrow \frac{1}{\delta_r} y_r$; compatible $\leftarrow 1$;
else
compatible $\leftarrow 0$;
end if

The following small example is chosen to illustrate Algorithm 3.1, with our choices for $\theta_k > 0$, q_{tol} and δ_{tol} , on a compatible case of (1.1) where H is a singular matrix. The example also illustrates the change of sign between δ_{k+1} and δ_{k-1} when $\delta_k = 0$.

Example 3.2. *Let*

$$c = \begin{pmatrix} 3 & 2 & 1 & 0 & -1 & -2 & -3 \end{pmatrix}^T, \quad H = \text{diag}(c),$$

Algorithm 3.1 applied to H and c with $\theta_k > 0$ such that $\|y_k\| = \|c\|$, $k = 1, \dots, r$, and $q_{tol} = \delta_{tol} = \sqrt{\epsilon_M}$, yields the following sequences

q =

3.0000	-9.0000	2.2678	-2.7046	0.2648	-0.2445	0.0000
2.0000	-4.0000	-2.2678	5.4912	-1.0591	1.4673	0
1.0000	-1.0000	-2.2678	2.3768	1.3239	-3.6681	0
0	0	0	0	0	0	0
-1.0000	-1.0000	2.2678	2.3768	-1.3239	-3.6681	0
-2.0000	-4.0000	2.2678	5.4912	1.0591	1.4673	0
-3.0000	-9.0000	-2.2678	-2.7046	-0.2648	-0.2445	-0.0000

$$y = \begin{pmatrix} 0 & -3.0000 & 3.4017 & -0.9015 & -2.2241 & -0.0815 & 2.1602 \\ 0 & -2.0000 & 1.5119 & 2.7456 & -2.8419 & 0.7336 & 2.1602 \\ 0 & -1.0000 & 0.3780 & 2.3768 & -0.9885 & -3.6681 & 2.1602 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0.3780 & -2.3768 & -0.9885 & 3.6681 & 2.1602 \\ 0 & 2.0000 & 1.5119 & -2.7456 & -2.8419 & -0.7336 & 2.1602 \\ 0 & 3.0000 & 3.4017 & 0.9015 & -2.2241 & 0.0815 & 2.1602 \end{pmatrix}$$

$$\text{delta} = \begin{pmatrix} 1.0000 & 0 & -2.6458 & 0 & 2.3123 & 0 & -2.1602 \end{pmatrix}$$

Hence, $r = 6$ and $x_r = (1/\delta_r)y_r = \begin{pmatrix} -1 & -1 & -1 & 0 & -1 & -1 & -1 \end{pmatrix}^T$.

An example of an incompatible system will be given in Section 4.2.

3.3. On the case when normalization is well defined

It is well-known that when normalization is well defined and applied to Algorithm 3.1, then the method of conjugate gradients, by Hestenes and Stiefel [17], is obtained. In this case, we denote (q_k, y_k, δ_k) , by $(g_k, x_k, 1)$ and the recursions for g_k and x_k simplify such that it is possible to obtain a two-term recurrence of a search-direction p_k . The normalization condition for θ_k is $\theta_k = 1/(\alpha_k + \beta_{k-1})$. We show in Proposition A.6 that this choice for θ_k corresponds exactly to the optimal step-length along p_k , which was the motivation for setting up the recursion (2.2) on that particular form.

In Lemma A.5, we show that if $H \succeq 0$ then $\delta_i \neq 0$, for $i = 0, \dots, r-1$. Also, if $\delta_k > 0$ and $\delta_{k+1} \neq 0$, then $\delta_{k+1} > 0$ if and only if $\theta_k > 0$. Hence, it holds that for $H \succeq 0$, $\theta_i > 0$, $i = 0, \dots, r-1$, and $\delta_0 > 0$, then $\delta_i > 0$, $i = 0, \dots, r-1$, and $\delta_r \geq 0$. With the additional information that $c \in \mathcal{R}(H)$ it holds that $\delta_r > 0$ and normalization is possible in every iteration. On the other hand for $H \succeq 0$, $\theta_i > 0$, $i = 0, \dots, r-1$, $\delta_0 > 0$ and $c \notin \mathcal{R}(H)$, then $\delta_r = 0$ and normalization is possible at all but the final iteration. Further, if $H \succ 0$ and $\theta_i > 0$, $i = 0, \dots, r-1$, then $\delta_i > 0$, $i = 1, \dots, r$, i.e., $\delta_r \neq 0$ since (1.1) with $H \succ 0$ is always compatible.

4. Connection to the minimum-residual method

In the case when (1.1) is incompatible, instead of just a certificate of this fact, one would often be interested in a vector x that is "as good as possible". The method of choice could then be the minimum residual method which will return a solution in the compatible case, and a minimum-residual solution in the incompatible case. This method goes back to Lanczos early paper [19] and Stiefel [28], and the name is adopted from the implementation of the method, MINRES, by Paige and Saunders, see [24].

For $k = 0, \dots, r$, x_k^{MR} is defined as a solution to $\min_{x \in \mathcal{K}_k(c, H)} \|Hx + c\|_2^2$, and the corresponding residual g_k^{MR} is defined as $g_k^{MR} = Hx_k^{MR} + c$. The vectors x_k^{MR} are uniquely defined for $k = 0, \dots, r-1$, and for $k = r$ if $c \in \mathcal{R}(H)$. For the

case $k = r$ and $c \notin \mathcal{R}(H)$ there is one degree of freedom for x_r^{MR} . If $c \in \mathcal{R}(H)$, then x_r^{MR} solves (1.1), and if $c \notin \mathcal{R}(H)$, then x_{r-1}^{MR} and x_r^{MR} are both solutions to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$.

4.1. Convergence of the minimum-residual method

In the following theorem, we derive the minimum-residual method based on the unnormalized Krylov subspace framework. In particular, we give explicit formulas for x_k^{MR} and g_k^{MR} , $k = 0, \dots, r$. For the case $k = r$, $c \notin \mathcal{R}(H)$, we give an explicit formula for x_r^{MR} of minimum Euclidean norm.

Theorem 4.1. *Let (q_k, y_k, δ_k) be given by Lemma 2.2 for $k = 0, \dots, r$. Then, for $k = 0, \dots, r$, it holds that x_k^{MR} solves $\min_{x \in \mathcal{K}_k(c, H)} \|Hx + c\|_2^2$ if and only if $x_k^{MR} = \sum_{i=0}^k \gamma_i y_i$ for some γ_i , $i = 0, \dots, k$, that are optimal to*

$$\begin{aligned} & \underset{\gamma_0, \dots, \gamma_k}{\text{minimize}} \quad \frac{1}{2} \sum_{i=0}^k \gamma_i^2 q_i^T q_i \\ & \text{subject to} \quad \sum_{i=0}^k \gamma_i \delta_i = 1. \end{aligned} \quad (4.1)$$

In particular, x_k^{MR} takes the following form for the mutually exclusive cases (a) $k < r$; (b) $k = r$ and $\delta_r \neq 0$; and (c) $k = r$ and $\delta_r = 0$.

a) For $k < r$, it holds that

$$x_k^{MR} = \frac{1}{\sum_{j=0}^k \frac{\delta_j^2}{q_j^T q_j}} \sum_{i=0}^k \frac{\delta_i}{q_i^T q_i} y_i, \quad (4.2)$$

and $g_k^{MR} = Hx_k^{MR} + c \neq 0$.

b) For $k = r$ and $\delta_r \neq 0$, it holds that $x_r^{MR} = (1/\delta_r)y_r$ and $g_r^{MR} = Hx_r^{MR} + c = 0$, so that x_r^{MR} solves (1.1) and x_r^{MR} is identical to x_r of Theorem 3.1.

c) For $k = r$ and $\delta_r = 0$, it holds that $x_r^{MR} = x_{r-1}^{MR} + \gamma_r y_r$, where γ_r is an arbitrary scalar, and $g_r^{MR} = Hx_r^{MR} + c = g_{r-1}^{MR} \neq 0$. In addition, x_{r-1}^{MR} and x_r^{MR} solve $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$. The particular choice

$$\gamma_r = -\frac{y_r^T x_{r-1}^{MR}}{y_r^T y_r}$$

makes x_r^{MR} an optimal solution to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$ of minimum Euclidean norm.

Proof. Since q_i , $i = 0, \dots, k$, form an orthogonal basis for $\mathcal{K}_{k+1}(c, H)$, an arbitrary vector in $\mathcal{K}_{k+1}(c, H)$ can be written as

$$g = \sum_{i=0}^k \gamma_i q_i = \sum_{i=0}^k \gamma_i (Hy_i + \delta_i c) = H \left(\sum_{i=0}^k \gamma_i y_i \right) + \left(\sum_{i=0}^k \gamma_i \delta_i \right) c, \quad (4.3)$$

for some parameters γ_i , $i = 0, \dots, k$. Consequently, the condition $\sum_{i=0}^k \gamma_i \delta_i = 1$ inserted into (4.3) gives $g = Hx + c$ with $x = \sum_{i=0}^k \gamma_i y_i$, i.e., g is an arbitrary vector in $\mathcal{K}_{k+1}(c, H)$ for which the coefficient in front of c equals one, and x is the corresponding arbitrary vector in $\mathcal{K}_k(c, H)$. Minimizing the Euclidean norm of such a g gives the quadratic program

$$\begin{aligned} & \underset{g, \gamma_0, \dots, \gamma_k}{\text{minimize}} && \frac{1}{2} g^T g \\ & \text{subject to} && g = \sum_{i=0}^k \gamma_i q_i, \\ & && \sum_{i=0}^k \gamma_i \delta_i = 1, \end{aligned} \tag{4.4}$$

so that, by (4.3), the optimal values of γ_i , $i = 0, \dots, k$, give g_k^{MR} as $g_k^{MR} = \sum_{i=0}^k \gamma_i q_i$ and x_k^{MR} as $x_k^{MR} = \sum_{i=0}^k \gamma_i y_i$. Elimination of g in (4.4), taking into account the orthogonality of the q_i 's, gives the equivalent problem (4.1). Also note that since $\delta_0 \neq 0$, the quadratic programs (4.1) and (4.4) are always feasible, and hence they are well defined.

Let $\mathcal{L}(\gamma, \lambda)$ be the Lagrangian function for (4.1),

$$\mathcal{L}(\gamma, \lambda) = \frac{1}{2} \sum_{i=0}^k \gamma_i^2 q_i^T q_i - \lambda \left(\sum_{i=0}^k \gamma_i \delta_i - 1 \right).$$

The optimality conditions for (4.1) are given by

$$0 = \nabla_{\gamma_i} \mathcal{L}(\gamma, \lambda) = \gamma_i q_i^T q_i - \lambda \delta_i, \quad i = 0, \dots, k, \tag{4.5a}$$

$$0 = \nabla_{\lambda} \mathcal{L}(\gamma, \lambda) = 1 - \sum_{i=0}^k \gamma_i \delta_i. \tag{4.5b}$$

First, for (a), consider the case $k < r$. From (4.5a) it holds that

$$\gamma_i = \lambda \frac{\delta_i}{q_i^T q_i}, \quad i = 0, \dots, k, \tag{4.6}$$

which are well defined, since $q_i \neq 0$, $i = 0, \dots, r-1$. The expression for λ is obtained by inserting the expression for γ_i , $i = 0, \dots, k$, given by (4.6) in (4.5b) so that

$$1 = \sum_{i=0}^k \gamma_i \delta_i = \sum_{i=0}^k \lambda \frac{\delta_i^2}{q_i^T q_i} \quad \text{yielding} \quad \lambda = \frac{1}{\sum_{i=0}^k \frac{\delta_i^2}{q_i^T q_i}}. \tag{4.7}$$

Consequently, a combination of (4.6) and (4.7) gives

$$\gamma_i = \frac{1}{\sum_{j=0}^k \frac{\delta_j^2}{q_j^T q_j}} \frac{\delta_i}{q_i^T q_i}, \quad i = 0, \dots, k. \tag{4.8}$$

Hence, by letting $x_k^{MR} = \sum_{i=0}^k \gamma_i y_i$, with γ_i given by (4.8), (4.2) follows.

Now, for (b), consider the case $k = r$ with $\delta_r \neq 0$. Then, since $q_r = 0$, (4.5a) gives $\lambda = 0$ and $\gamma_i = 0$, $i = 0, \dots, r-1$. Consequently, (4.5b) gives $\gamma_r = 1/\delta_r$.

Again, by letting $x_r^{MR} = \sum_{i=0}^r \gamma_i y_i$, it holds that $x_k^{MR} = (1/\delta_r) y_r$, for which $g_k^{MR} = Hx_k^{MR} + c = 0$, so that the optimal value is zero in (4.1) and x_r^{MR} solves (1.1).

Finally, for (c), consider the case $k = r$ with $\delta_r = 0$. Theorem 3.1 shows that there exists an $x_r^{(1)} \in \mathcal{K}_{r-1}(c, H)$ that solves $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$. Consequently, since $x_r^{(1)} \in K_{r-1}(c, H)$, it follows from (a) that it must hold that $x_r^{(1)} = x_{r-1}^{MR}$ so that x_{r-1}^{MR} solves $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$.

For $k = r$, the optimality conditions (4.5) are equivalent to when $k = r - 1$, just with the additional information that γ_r is arbitrary. Hence, $x_r^{MR} = x_{r-1}^{MR} + \gamma_r y_r$ and $g_r^{MR} = Hx_r^{MR} + c = g_{r-1}^{MR}$ for arbitrary γ_r since $Hy_r = 0$.

Regardless of the value of γ_r , the range-space component of x_r^{MR} is unique, since Theorem 3.1 gives $Hy_r = 0$. For the remainder of the proof, let $x_r^{MR} = x_{r-1}^{MR} + \gamma_r y_r$ for the particular choice $\gamma_r = -(y_r^T x_{r-1}^{MR}) / (y_r^T y_r)$, so that $y_r^T x_r^{MR} = 0$. We will show that for this particular choice the null-space component of x_r^{MR} is zero, and hence x_r^{MR} is an optimal solution to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$ of minimum Euclidean norm.

Since $y_k = Hy_k^{(1)} + \delta_k^{(1)} c$, it follows that $Z^T y_k = \delta_k^{(1)} Z^T c$, $k = 0, \dots, r$. Consequently, since x_r^{MR} is formed as a linear combination of y_k , $k = 0, \dots, r$, it holds that $Z^T x_r^{MR}$ is parallel to $Z^T c$. But $0 = y_r^T x_r^{MR} = (\delta_r^{(1)} Z^T c)^T Z^T x_r^{MR} = 0$, so that $Z^T x_r^{MR}$ is also orthogonal to $Z^T c$. By Theorem 3.1, $\delta_r^{(1)} \neq 0$ and $Z^T c \neq 0$, so that $Z^T x_r^{MR} = 0$. Hence, the null space component of x_r^{MR} is zero. ■

Note that at an iteration k at which $\delta_k = 0$ and $q_k \neq 0$, it holds that $x_k^{MR} = x_{k-1}^{MR}$ so that the iterate is unchanged. This is referred to as stagnation, and in accordance with Brown [3] it holds that the unnormalized Krylov method and the minimum-residual method form a pair, see, e.g., [26, Proposition 6.17]. In the framework of this paper, it holds that normalization is not possible at step k in the Krylov method if and only if there is stagnation in the minimum-residual method. Note that this cannot happen at two consecutive iterations. If $q_k \neq 0$, all information from the problem has not been extracted even if $\delta_k = 0$. Only in the case when $k = r$, global information is obtained, and it is determined whether (1.1) has a solution or not.

In the following corollary of Theorem 4.1 we state explicit recursions for the minimum-residual method.

Corollary 4.2. *Let (q_k, y_k, δ_k) be given by Lemma 2.2 and let x_k^{MR} be given by Theorem 4.1 for $k = 0, \dots, r$. If $\delta_0^{MR} = \delta_0^2$, $y_0^{MR} = \delta_0 y_0$,*

$$\delta_k^{MR} = q_k^T q_k \sum_{i=0}^{k-1} \frac{\delta_i^2}{q_i^T q_i} + \delta_k^2 \quad \text{and} \quad y_k^{MR} = q_k^T q_k \sum_{i=0}^{k-1} \frac{\delta_i}{q_i^T q_i} y_i + \delta_k y_k, \quad k = 1, \dots, r,$$

then

$$x_k^{MR} = \frac{1}{\delta_k^{MR}} y_k^{MR}, \quad k = 0, \dots, r-1 \quad \text{and} \quad k = r \text{ if } \delta_r \neq 0.$$

In addition, it holds that

$$\delta_{k+1}^{MR} = \frac{q_{k+1}^T q_{k+1}}{q_k^T q_k} \delta_k^{MR} + \delta_{k+1}^2 \quad \text{and} \quad y_{k+1}^{MR} = \frac{q_{k+1}^T q_{k+1}}{q_k^T q_k} y_k^{MR} + \delta_{k+1} y_{k+1},$$

for $k = 0, \dots, r-1$.

Proof. For $k = 0, \dots, r-1$, the expressions for δ_k^{MR} and y_k^{MR} give

$$\frac{1}{q_k^T q_k} \delta_k^{MR} = \sum_{i=0}^k \frac{\delta_i^2}{q_i^T q_i} \quad \text{and} \quad \frac{1}{q_k^T q_k} y_k^{MR} = \sum_{i=0}^k \frac{\delta_i}{q_i^T q_i} y_i.$$

Note that $\delta_0 \neq 0$ and $q_i \neq 0$, $i = 0, \dots, k$ implies $\delta_k^{MR} > 0$ for $k < r$. Hence, Theorem 4.1 gives $x_k^{MR} = (1/\delta_k^{MR})y_k^{MR}$. If $k = r$ and $\delta_r \neq 0$, the expressions for δ_r^{MR} and y_r^{MR} give

$$\delta_r^{MR} = \delta_r^2 > 0 \quad \text{and} \quad y_r^{MR} = \delta_r y_r,$$

so that Theorem 4.1 gives $x_r^{MR} = (1/\delta_r^{MR})y_r^{MR}$ also for this case.

The recursions for y_{k+1}^{MR} and δ_{k+1}^{MR} , $k = 0, \dots, r-1$, are straightforward to obtain.

■

The recursion for x_r^{MR} , based on x_{r-1}^{MR} and (q_r, y_r, δ_r) , for the case $\delta_r = 0$ is given in Theorem 4.1 and it is not reiterated in Corollary 4.2.

Note that the expressions in Theorem 4.1 and Corollary 4.2 for x_k^{MR} , $k = 0, \dots, r$, are independent of the scaling of (q_k, y_k, δ_k) . Hence, if $H \succeq 0$ and $c \in \mathcal{R}(H)$ then normalization is well defined so that $(g_k, x_k, 1)$ may be used to give x_k^{MR} , $k = 0, \dots, r-1$, as convex combinations of x_i , $i = 0, \dots, k$, respectively.

4.2. A minimum-residual algorithm based on the unnormalized Krylov method

To summarize we next state an algorithm for the minimum-residual method based on Algorithm 3.1 and extended with the recursions in Corollary 4.2.

Algorithm 4.2 A minimum-residual algorithm based on the unnormalized Krylov method

Input arguments: H, c ;

Output arguments: x_r^{MR}, g_r^{MR} , compatible; (x_r or y_r if compatible=1 or 0);

Run Algorithm 3.1 with the extra initialization

$$y_0^{MR} \leftarrow \delta_0 y_0; \quad \delta_0^{MR} \leftarrow \delta_0^2; \quad x_0^{MR} \leftarrow \frac{1}{\delta_0^{MR}} y_0^{MR}; \quad g_0^{MR} \leftarrow H x_0^{MR} + c;$$

For $k = 1$ calculate in addition

$$y_1^{MR} \leftarrow \frac{q_1^T q_1}{q_0^T q_0} y_0^{MR} + \delta_1 y_1; \quad \delta_1^{MR} \leftarrow \frac{q_1^T q_1}{q_0^T q_0} \delta_0^{MR} + \delta_1^2;$$

$$x_1^{MR} \leftarrow \frac{1}{\delta_1^{MR}} y_1^{MR}; \quad g_1^{MR} \leftarrow H x_1^{MR} + c;$$

For $k > 1$ until termination calculate in addition

$$y_{k+1}^{MR} \leftarrow \frac{q_{k+1}^T q_{k+1}}{q_k^T q_k} y_k^{MR} + \delta_{k+1} y_{k+1}; \quad \delta_{k+1}^{MR} \leftarrow \frac{q_{k+1}^T q_{k+1}}{q_k^T q_k} \delta_k^{MR} + \delta_{k+1}^2;$$

$$x_{k+1}^{MR} \leftarrow \frac{1}{\delta_{k+1}^{MR}} y_{k+1}^{MR}; \quad g_{k+1}^{MR} \leftarrow H x_{k+1}^{MR} + c;$$

At termination, if $|\delta_r| < \delta_{tol}$, calculate in addition

$$x_r^{MR} \leftarrow x_{r-1}^{MR} - \frac{y_{r-1}^{MR}}{y_r^T y_r} y_r; \quad \text{compatible} \leftarrow 0;$$

Hence, for a compatible system (1.1) Algorithm 4.2 gives the same solution x_r as Algorithm 3.1, and in addition it calculates x_r^{MR} . They are both estimates of a

solution to (1.1). Further, if (1.1) is incompatible then Algorithm 4.2 delivers x_r^{MR} , an optimal solution to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$ of minimum Euclidean norm, in addition to the certificate of incompatibility.

Next we observe another small example chosen to illustrates Algorithm 4.2 with our choices for $\theta_k > 0$, q_{tol} and δ_{tol} , on a case when (1.1) is incompatible, i.e. $c \notin \mathcal{R}(H)$.

Example 4.3. *Let*

$$c = \begin{pmatrix} 3 & 2 & 1 & 1 & -1 & -2 & -3 \end{pmatrix}^T, \quad H = \text{diag} \begin{pmatrix} 5 & 2 & 1 & 0 & -1 & -2 & -3 \end{pmatrix},$$

Algorithm 4.2 applied to H and c with $\theta_k > 0$ such that $\|y_k\| = \|c\|$, $k = 1, \dots, r$, and $q_{tol} = \delta_{tol} = \sqrt{\epsilon_M}$, yields the following sequences

q =

3.0000	-13.1379	3.5628	-0.8597	0.1063	-0.0181	0.0017	-0.0000
2.0000	-2.7586	-5.7676	3.9832	-1.3787	0.6372	-0.1470	-0.0000
1.0000	-0.3793	-3.1464	0.1039	1.8638	-2.5737	1.1021	0.0000
1.0000	0.6207	-2.8617	-1.7605	2.2573	0.5896	-1.7634	-0.0000
-1.0000	-1.6207	2.0296	2.7934	-0.6882	-2.4489	-1.4695	0.0000
-2.0000	-5.2414	1.3007	4.3735	2.1842	1.1548	0.3149	-0.0000
-3.0000	-10.8621	-3.8286	-2.6032	-0.6658	-0.2082	-0.0367	0.0000

y =

0	-3.0000	2.4296	0.8844	-1.3331	-0.3574	1.0584	-0.0000
0	-2.0000	-0.0222	3.7521	-2.9466	-0.2710	1.6899	0
0	-1.0000	-0.2847	1.8644	-0.3935	-3.1633	2.8655	0.0000
0	-1.0000	-0.5584	1.5833	0.7502	-3.7018	-0.7931	5.3852
0	1.0000	0.8320	-1.0329	-1.5691	1.8593	3.2329	0.0000
0	2.0000	2.2113	-0.4262	-3.3494	-1.1670	1.6060	0.0000
0	3.0000	4.1379	2.6283	-2.0353	-0.5202	1.7756	0.0000

delta =

1.0000	0.6207	-2.8617	-1.7605	2.2573	0.5896	-1.7634	-0.0000
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xMR =

0	-0.1588	-0.6633	-0.6143	-0.5995	-0.5998	-0.6000	-0.6000
0	-0.1059	-0.0228	-0.6647	-1.0640	-1.0371	-1.0000	-1.0000
0	-0.0529	0.0585	-0.2817	-0.2148	-0.4441	-1.0000	-1.0000
0	-0.0529	0.1284	-0.1845	0.1376	-0.1481	0.1333	-0.0000
0	0.0529	-0.1983	0.0407	-0.4178	-0.2588	-1.0000	-1.0000
0	0.1059	-0.5364	-0.2994	-1.0375	-1.0794	-1.0000	-1.0000
0	0.1588	-1.0143	-1.1600	-0.9990	-0.9938	-1.0000	-1.0000

Hence, $r = 7$ and $x_r^{MR} = \begin{pmatrix} -0.6 & -1 & -1 & 0 & -1 & -1 & -1 \end{pmatrix}^T$. Note that, since $|\delta_r| < \delta_{tol}$, the system is considered incompatible and x_r^{MR} is the optimal solution to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$ of minimum Euclidean norm and $\|Hx_r^{MR} + c\|_2^2 = 1$.

5. Summary and conclusion

By making use of an unnormalized Krylov subspace framework for solving symmetric system of linear equations, as proposed by Gutknecht [11, 12], we show how to determine, in exact arithmetic, if the system is compatible or incompatible. In the compatible case, a solution is given. In the incompatible case, a certificate of incompatibility is obtained. The basis of this framework are the triples (q_k, y_k, δ_k) , $k = 0, \dots, r$, given by Lemma 2.2, that are uniquely defined up to a scaling. Our results include and handle the case of a singular matrix H . To the best of our knowledge this is not covered in any previous work.

We have also put the minimum-residual method in this framework and provided explicit formulas for the iterations. Again, the analysis is based on the triples. In the case of an incompatible system, our analysis gives an expression for x_r^{MR} of minimum Euclidean norm. The original implementation of MINRES by Paige and Saunders, [24], did not deliver the optimal solution to $\min_{x \in \mathbb{R}^n} \|Hx + c\|_2^2$ of minimum Euclidean norm. In [5], Choi, Paige and Saunders present a MINRES-like algorithm, MINRES-QLP, that does.

One may observe that an alternative to using the minimum-residual iterations would be to consider recursions for $y_k^{(1)}$ and $\delta_k^{(1)}$ as given by (2.8) and then calculate $x_{r-1}^{MR} = (1/\delta_r^{(1)})y_r^{(1)}$, according to the analysis in the proof of Theorems 3.1 and 4.1. However, such an approach would not automatically yield the estimates x_k^{MR} , $k = 0, \dots, r-2$.

One could also note that the method of conjugate gradients may be viewed as trying to solve the minimum-residual problem (4.1) in the situation where only the present triple (q_k, y_k, δ_k) is allowed in the linear combination, i.e., $\gamma_i = 0$, $i = 0, \dots, k-1$. This problem is then not necessarily feasible. It will be infeasible exactly when $\delta_k = 0$. One could think of methods other than the minimum-residual method which use a linear combination of more than one triple. It would suffice to use two consecutive triples, since it cannot hold that $\delta_{k-1} = 0$ and $\delta_k = 0$.

Finally, we want to stress that this paper is meant to give insight into the unnormalized Krylov subspace framework, in exact arithmetic. In finite precision, the unnormalized Krylov method would inherit deficiencies of any method based on a Lanczos process such as loss of orthogonality of the generated vectors. It is beyond the scope of the present paper to make such an analysis, see, e.g., [16, 21, 22, 25]. The theory of our paper is based on determining if certain quantities are zero or not. In our algorithms, we have made choices on optimality tolerances that are not meant to be universal. To obtain a fully functioning algorithm, the issue of determining if a quantity is near-zero would need to be considered more in detail. Also, we have based our analysis on the triples, so that termination of Algorithm 4.2 is based on q_k and δ_k . In practice, one should probably also consider g_k^{MR} .

Further, the use of pre-conditioning is not explored in this paper, for this subject see, e.g., [1, 6, 7].

A. Appendix

A.1. A result on the Lanczos vectors

For completeness, we review a result that characterizes the properties of q_k expressed as in (2.1), needed for the analysis.

Lemma A.1. *Let r denote the smallest positive integer k for which $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$. For an index k such that $1 \leq k \leq r$, let $q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp$, be expressed as in (2.1). Then, the scalars $\delta_k^{(j)}$, $j = 0, \dots, k$, are uniquely determined up to a nonzero scaling. In addition, if $\delta_k^{(k)} \neq 0$ it holds that $q_k = 0$ if and only if $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$, i.e., if $k = r$.*

Proof. Assume that $q_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp$ is expressed as in (2.1). If $k < r$, then $c, Hc, H^2c, \dots, H^k c$ are linearly independent. Hence, $\delta_k^{(j)}$, $j = 0, \dots, k$, are uniquely determined by q_k . Consequently, as q_k is uniquely defined up to a nonzero scaling, then so are $\delta_k^{(j)}$, $j = 0, \dots, k$. For $k = r$, we have $q_r = 0$ so that

$$-\delta_r^{(r)} H^r c = \sum_{j=0}^{r-1} \delta_r^{(j)} H^j c. \quad (\text{A.1})$$

By the definition of r , it holds that $c, Hc, H^2c, \dots, H^{r-1}c$ are linearly independent. Hence, (A.1) shows that a fixed $\delta_r^{(r)}$ uniquely determines $\delta_r^{(j)}$, $j = 1, \dots, r-1$. Consequently, a scaling of $\delta_r^{(r)}$ gives a corresponding scaling of $\delta_r^{(j)}$, $j = 0, \dots, r-1$. Thus, $\delta_r^{(j)}$, $j = 0, \dots, r$, are uniquely determined up to a common scaling.

Finally, assume that $\delta_k^{(k)} \neq 0$. By definition $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$ implies $q_k = 0$. To show the converse, assume that $q_k = 0$. Then,

$$-\delta_k^{(k)} H^k c = \sum_{j=0}^{k-1} \delta_k^{(j)} H^j c. \quad (\text{A.2})$$

If $\delta_k^{(k)} \neq 0$, then (A.2) implies $H^k c \in \text{span}\{c, Hc, H^2c, \dots, H^{k-1}c\}$, i.e., $\mathcal{K}_{k+1}(c, H) = \mathcal{K}_k(c, H)$, completing the proof. ■

A.2. Properties of the sequence $\{\delta_k\}$

In the following proposition it is shown that the sequence $\{\delta_k\}$ can not have two zero elements in a row.

Proposition A.2. *Let (q_k, y_k, δ_k) , $k = 0, \dots, r$, be given by Lemma 2.2. If $q_k \neq 0$ and $\delta_k = 0$, then*

$$\delta_{k+1} = -\frac{\theta_k}{\theta_{k-1}} \frac{q_k^T q_k}{q_{k-1}^T q_{k-1}} \delta_{k-1} \neq 0.$$

Proof. By Proposition 2.1 it holds that

$$q_k^T q_k = -\theta_{k-1} q_k^T H q_{k-1},$$

and, taking into account $\delta_k = 0$, the expression for δ_{k+1} from Proposition 2.2 gives

$$\delta_{k+1} = \theta_k \frac{q_{k-1}^T H q_k}{q_{k-1}^T q_{k-1}} \delta_{k-1} = -\frac{\theta_k}{\theta_{k-1}} \frac{q_k^T q_k}{q_{k-1}^T q_{k-1}} \delta_{k-1}, \quad (\text{A.3})$$

giving the required expression for δ_{k+1} .

It remains to show that $\delta_{k+1} \neq 0$. First, assume that $k = 1$ so that $\delta_1 = 0$. Then, since $\theta_1 \neq 0$, $\theta_0 \neq 0$ and $\delta_0 = 1$, (A.3) gives $\delta_2 \neq 0$. Now assume that $k > 1$. Assume, to get a contradiction, that $\delta_{k+1} = 0$. Then, since $\theta_k \neq 0$, $\theta_{k-1} \neq 0$, (A.3) gives $\delta_{k-1} = 0$. We may then repeat the same argument to obtain $\delta_i = 0$, $i = 1, \dots, k$. But this gives a contradiction, as $\delta_1 = 0$ implies $\delta_2 \neq 0$. Hence, it must hold that $\delta_{k+1} \neq 0$, as required. ■

Based on Proposition A.2 the following corollary states that if θ_{k-1} and θ_k have the same sign and $\delta_k = 0$, then δ_{k+1} and δ_{k-1} will have opposite signs.

Corollary A.3. *Let (q_k, y_k, δ_k) , $k = 0, \dots, r$, be given by Proposition 2.2 with θ_{k-1} and θ_k of the same sign. If $q_k \neq 0$ and $\delta_k = 0$, then $\delta_{k+1} \delta_{k-1} < 0$.*

The following lemma states an expression for the triples that is used in showing properties of the signs of δ_k and θ_k for the case when H is positive semidefinite.

Lemma A.4. *Let (q_k, y_k, δ_k) , $k = 0, \dots, r$, be given by Lemma 2.2. If $\delta_k \neq 0$ and $k < r$, then*

$$(y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T H (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k) = \theta_k \frac{\delta_{k+1}}{\delta_k} q_k^T q_k. \quad (\text{A.4})$$

Proof. Eliminating c from the difference of q_{k+1} and q_k yields

$$q_{k+1} - \frac{\delta_{k+1}}{\delta_k} q_k = H (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k). \quad (\text{A.5})$$

Then pre-multiplication of (A.5) with $(y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T$ yields

$$(y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T (q_{k+1} - \frac{\delta_{k+1}}{\delta_k} q_k) = (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T H (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k). \quad (\text{A.6})$$

Since q_{k+1} is orthogonal to y_{k+1} and y_k , and since q_k is orthogonal to y_k , (A.6) becomes

$$-\frac{\delta_{k+1}}{\delta_k} y_{k+1}^T q_k = (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T H (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k). \quad (\text{A.7})$$

Hence, by Proposition 2.1 and since q_k is orthogonal to y_k and y_{k-1} , (A.7) may be written as

$$\theta_k \frac{\delta_{k+1}}{\delta_k} q_k^T q_k = (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k)^T H (y_{k+1} - \frac{\delta_{k+1}}{\delta_k} y_k),$$

hence (A.4) is obtained. ■

The following lemma gives some results on the behavior of the sequence of $\{\delta_k\}$ in connection to the sign of θ_k for the case when $H \succeq 0$.

Lemma A.5. *Let (q_k, y_k, δ_k) , $k = 0, \dots, r$, be given by Lemma 2.2. Assume that $H \succeq 0$. Then $\delta_k \neq 0$ for $k < r$. If $\delta_k > 0$ and $\delta_{k+1} \neq 0$, then $\delta_{k+1} > 0$ if and only if $\theta_k > 0$.*

Proof. Assume that $\delta_k = 0$ for $k < r$, then $q_k = Hy_k$, hence pre-multiplication with y_k^T yields $0 = y_k^T q_k = y_k^T Hy_k$, since q_k is orthogonal to y_k . Then, since $H \succeq 0$, it follows that $Hy_k = 0$ and hence $q_k = 0$. Since $q_k \neq 0$ for $k < r$, the assumption yields a contradiction. Hence, $\delta_k \neq 0$, $k < r$.

Next suppose that $\delta_k > 0$ and $\delta_{k+1} \neq 0$. Since $H \succeq 0$, Lemma A.4 gives

$$\theta_k \frac{\delta_{k+1}}{\delta_k} q_k^T q_k \geq 0, \quad (\text{A.8})$$

which implies that δ_{k+1} and δ_k have the same sign if and only if $\theta_k > 0$. Hence, if $\delta_k > 0$, then $\delta_{k+1} > 0$ if and only if $\theta_k > 0$. ■

The relation of the signs in Lemma A.5 is a consequence of our choice of the minus-sign in (2.4). Otherwise δ_k would alternate sign in each iteration for $\theta_k > 0$ and $H \succeq 0$.

A consequence of Lemma A.5 is that if θ_k is chosen positive for $k = 0, \dots, r$, then $\delta_k \leq 0$ for some k implies $H \not\succeq 0$ and $\delta_k < 0$ for some k implies $H \not\preceq 0$.

A.3. The method of conjugate gradients

If normalization is well defined and applied to Algorithm 3.1, then one obtains the method of conjugate gradients, by Hestenes and Stiefel [17]. For an introduction to the method of conjugate gradients see, e.g., [20, 27]. This method is usually defined for the case where $H \succ 0$. In the method of conjugate gradients, an iterate x_k is defined as the solution to $\min_{\mathcal{K}_k(c, H)} \frac{1}{2} x^T H x + c^T x$, and $g_k = Hx_k + c$ for $k = 0, \dots, r$, i.e., $g_k \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp$.

In the setting of this paper, it is equivalent to generating triples (q_k, y_k, δ_k) , $k = 0, \dots, r$, given by Lemma 2.2, selecting the scaling θ_k in (2.9) such that $\delta_k = 1$, for all k . With the additional assumption $H \succeq 0$, Lemma A.5 gives $\delta_k \neq 0$, $k = 0, \dots, r - 1$. If $c \in \mathcal{R}(H)$, i.e., (1.1) is compatible, then Theorem 3.1 ensures that also $\delta_r \neq 0$. Further, if $H \succeq 0$ and $c \notin \mathcal{R}(H)$, normalization will be well defined in all except the very last iteration.

For completeness, in the following proposition we show that when the normalization condition is satisfied, θ_k is exactly the step-length along the search-direction p_k in iteration k , so that the usual line-search description of the method of conjugate gradients, see, e.g., [26], follows.

Proposition A.6. Assume that $H \succeq 0$ and $c \in \mathcal{R}(H)$. If (q_k, y_k, δ_k) , $k = 0, \dots, r$, are given by Lemma 2.2, for the choice of θ_k in (2.9), then $\delta_k = 1$, $k = 1, \dots, r$, and $\theta_k > 0$, $k = 0, \dots, r-1$. Hence, denoting (q_k, y_k, δ_k) by $(g_k, x_k, 1)$, for

$$p_0 = -g_0, \quad p_k = -g_k + \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} p_{k-1}, \quad k = 1, \dots, r-1.$$

it holds that

$$x_{k+1} = x_k + \theta_k p_k, \quad k = 0, \dots, r-1,$$

$$g_{k+1} = g_k + \theta_k H p_k, \quad k = 0, \dots, r-1,$$

and further,

$$\theta_k = -\frac{g_k^T p_k}{p_k^T H p_k}, \quad k = 0, \dots, r-1.$$

Proof. Let $(q_0, y_0, \delta_0) = (c, 0, 1)$, then with θ_k as in (2.9), i.e.,

$$\theta_0 = \frac{1}{\alpha_0}, \quad \theta_k = \frac{1}{\alpha_k + \beta_{k-1}}, \quad k = 1, \dots, r-1,$$

where α_k , $k = 0, \dots, r-1$, and β_{k-1} , $k = 1, \dots, r-1$, are given by (2.5), the recursions of Lemma 2.2 yield $\delta_k = 1$, $k = 0, \dots, r-1$. Hence, by Lemma A.5, $\theta_k > 0$, $k = 0, \dots, r-1$. Denoting (q_k, y_k, δ_k) by $(g_k, x_k, 1)$, the recursions for x_k and g_k of Lemma 2.2 are then given by

$$\begin{aligned} x_1 &= x_0 + \theta_0(-g_0), \\ x_{k+1} &= x_k + \theta_k(-g_k - \beta_{k-1}(x_k - x_{k-1})), \quad k = 1, \dots, r-1, \end{aligned}$$

and

$$\begin{aligned} g_1 &= Hx_1 + c = g_0 + \theta_0(-Hg_0), \\ g_{k+1} &= Hx_{k+1} + c = g_k + \theta_k(-Hg_k - \beta_{k-1}(g_k - g_{k-1})), \quad k = 1, \dots, r-1. \end{aligned}$$

For $p_k = (1/\theta_k)(x_{k+1} - x_k)$, $k = 0, \dots, r-1$, the above recursions give

$$p_0 = -g_0, \quad \text{and} \quad p_k = -g_k - \beta_{k-1}(x_k - x_{k-1}), \quad k = 1, \dots, r-1.$$

By Proposition 2.1 it holds that $g_k^T g_k = -\theta_{k-1} g_k^T H g_{k-1}$, and therefore,

$$\beta_{k-1} = \frac{g_{k-1}^T H g_k}{g_{k-1}^T g_{k-1}} = -\frac{1}{\theta_{k-1}} \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}},$$

hence

$$p_k = -g_k - \beta_{k-1} \theta_{k-1} p_{k-1} = -g_k + \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} p_{k-1}, \quad k = 1, \dots, r-1.$$

Consequently, since $g_{k+1} - g_k = H(x_{k+1} - x_k) = \theta_k H p_k$, $k = 0, \dots, r-1$, it holds that $g_{k+1} = g_k + \theta_k H p_k$, $k = 0, \dots, r-1$. Further, $g_{k+1}^T p_k = 0$ since $g_{k+1} \in \mathcal{K}_{k+1}(c, H) \cap \mathcal{K}_k(c, H)^\perp$ and $p_k \in \mathcal{K}_k(c, H)$. Hence, $0 = g_{k+1}^T p_k = g_k^T p_k + \theta_k p_k^T H p_k$ yields

$$\theta_k = -\frac{g_k^T p_k}{p_k^T H p_k}, \quad k = 0, \dots, r-1,$$

completing the proof. ■

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